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Water Vapor Line Assignments in the Near Infrared

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The high-resolution spectrum of water vapor between 13 200 and 16 500 cm^{-1} recorded by J.-Y. Mandin, J-P. Chevillard, C. Camy-Peyret, J.-M. Flaud, and J. W. Brault (1986. *J. Molec. Spectrosc.*, **116,** 167) is analyzed using high-accuracy linelists obtained using ab initio calculations and spectroscopically determined potential. Assignments to $H_2{}^{16}O$ transitions are presented for 663 of the 795 unassigned lines presented in the original paper. In addition, 38 lines are reassigned. The majority of these assignments and reassignments are confirmed by combination differences. These assignments significantly extend the measured data for the 4ν and $4\nu + \delta$ polyads and provide the first information on the (240), (033), (160), (170), and (071) bands. It is likely that a significant fraction of the remaining unassigned lines belong to $H_2{}^{18}O$. © 1998 Academic Press

INTRODUCTION

Water is the major absorber of solar radiation in the earth's atmosphere. Yet at wavelengths covering the near infrared, visible, and ultraviolet, the spectrum of water remains poorly understood. In part this is because of the weakness of the water absorptions at these wavelengths, but spectra of water are also notoriously difficult to analyze. In particular, the most detailed observed water spectra in these regions (*1, 2*) contain many unassigned lines.

In this work we analyze the high-resolution water vapor spectrum of Mandin *et al.* (*2*). This spectrum was recorded using a Fourier transform spectrometer at the National Solar Observatory (Kitt Peak, Arizona) in the range 13 200–16 500 cm^{-1}. The spectrum contained 2796 transitions. Mandin *et al.* were able to assign 1927 of these to 17 $H_2{}^{16}O$ vibrational bands belonging to the 4ν and $4\nu + \delta$ polyads in their original work. A further 51 transitions were ascribed to $H_2{}^{18}O$; 769 lines remained unassigned.

Recently we have pioneered methods of analyzing spectra of hot water recorded both in the laboratory (*3–6*) and sunspots (*5–7*). In the present work we employ these methods to assign the majority of the unassigned lines in the spectrum of Mandin *et al.*

METHOD

Analysis was performed using two linelists, ZVPT (*6*) and PS (*8*). These linelists have both been generated using high-accuracy variational calculations for the vibration–rotation motion of the water. The major difference between the linelists is that ZVPT is based on ab initio calculations with explicit allowance made for non-Born–Oppenheimer effects (*9*), while the PS linelist used a potential that had been refined using spectroscopic data. Along with the two theoretical linelists, we also maintained a linelist generated using ''trivial'' transitions. Trivial transitions are ones that can be predicted accurately from known experimental energy levels. We started this linelist from Mandin *et al.*'s energy levels and PS's transition intensities. The linelist was continuously updated as new assignments were made using the calculated linelists.

Comparisons of the two theoretical linelists have been performed as part of our work on sunspot spectra (*6, 7*). The PS linelist is more accurate at estimating the frequency of individual transitions, particularly those with low J that concern us here. However the errors given by the PS linelist are often rather erratic. Conversely the ZVPT linelist is notable for giving very systematic errors, which allows one to make accurate predictions of the position of the next transition in a particular sequence or branch. The PS, but not the ZVPT, linelist contains a complete set of vibrational and rotational labels for each energy level and hence each transition. These are useful but must be treated with caution as the labels become increasing unreliable with excitation (*7*). For the upper states considered here about one-third of the labels proved to be incorrect. This problem appears to be particularly associated with representation of the normal mode–local mode behavior of 4ν and $4\nu + \delta$ water polyads. Thus most levels associated with (103) are labeled by PS as belonging to (301); similarly (122) levels are usually given as (320), and those with belonging to (113) as (311).

The spectrum of Mandin *et al.* (*2*) contains a considerable range of intensities. The strongest transitions show 100% peak absorption under the experimental conditions used, while there are many weak transitions with peak absorption of 0.5% or less. Mandin *et al.* assigned nearly all the strong

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TABLE 1

Newly Assigned Line Frequencies (in cm^{-1}) of the Near Infrared Water Vapor Spectrum of Mandin *et al.* (*2*).

ν (cm^{-1})	Intensity	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	
13245.4754	6	1	1	0	1	0	1	240	
13264.0965	4	6	3	3	7	5	2	221	a
13278.4710	5	2	1	2	1	0	1	240	
13299.2197	7	5	0	5	4	1	4	240	
13309.5095	4	6	4	2	7	6	1	301	a
13338.7866	7	11	1	11	12	1	12	221	
13341.8800	10	6	2	5	7	3	4	320	a
13347.4563	4	8	1	8	7	0	7	240	
13358.6682	4	7	1	6	8	4	5	202	a
13358.7600	5	6	1	5	5	2	4	240	
13366.8416	4	8	2	7	9	3	6	202	a
13367.2211	3	7	0	7	8	3	6	202	a,b
13369.5370	4	7	3	4	8	4	5	320	a
13370.0425	12	10	0	10	11	0	11	221	
13370.8576	6	10	1	10	11	1	11	221	a
13371.8090	3	2	2	1	1	1	0	240	
13372.1405	4	10	2	9	11	1	10	320	a
13373.5869	7								c
13381.6928	4	10	2	9	11	2	10	221	a
13384.3408	4	10	2	8	11	2	9	221	a
13385.2041	5	9	3	6	10	3	7	221	b
13386.7599	6	10	1	9	11	1	10	221	
13388.8116	6	7	1	6	6	2	5	240	
13400.7036	15	9	0	9	10	0	10	221	
13411.1724	18	9	3	7	10	3	8	221	
13411.8572	6	2	1	2	2	2	1	042	
13412.8430	5	5	3	2	6	4	3	320	a
13415.3367	9	8	3	6	9	0	9	240	a,b
13420.5980	13	8	0	8	9	2	7	071	a
13426.7960	6	9	5	4	10	5	5	301	
13433.4923	3	3	1	2	3	2	1	042	
13435.4400	6	7	2	5	8	5	4	122	a
13441.6289	10	5	2	3	6	3	4	320	a
13446.7153	10	7	1	7	8	2	6	170	a
13446.8864	12	8	3	6	9	2	7	320	a
13447.4087	8	7	3	5	8	1	8	141	a
13452.8875	31	7	0	7	8	1	8	320	b
13459.1757	5	6	3	4	6	4	3	042	a
13464.1761	38	7	5	2	8	2	7	160	a
13464.2476	10	2	1	1	3	3	0	221	
13466.5003	12	4	3	2	4	4	1	042	
13478.2882	6	6	0	6	7	1	7	320	a
13482.1160	15	5	1	4	6	2	5	320	a
13492.8370	5	7	0	7	7	1	6	320	a,b
13493.2951	31	6	4	3	7	1	6	240	a
13494.9680	90	6	1	5	7	3	4	301	a
13498.1457	6	4	1	3	5	2	4	320	a
13499.1390	4	6	2	5	7	3	4	202	a
13502.1741	23	9	2	7	10	3	8	202	a
13503.6623	11	5	0	5	6	1	6	320	a
13505.4007	6	8	4	5	9	3	6	320	a
13505.9251	20	10	1	9	11	2	10	202	a
13510.8741	5	6	4	3	7	2	6	141	a
13512.8020	5	4	4	0	5	2	3	141	a
13514.6152	8	3	1	2	4	2	3	320	a
13515.3407	7	7	6	1	7	7	0	202	a
13518.0045	18	5	2	4	6	1	5	320	a
13522.4182	16	8	5	3	9	5	4	221	a
13522.4606	17	6	3	4	7	2	5	320	a
13525.6350	5	7	1	6	7	3	5	221	a
13525.9328	17	4	4	1	5	5	0	202	a
13526.0917	7	8	3	6	8	4	5	320	a
13526.5757	7	4	0	4	5	1	5	320	a
13526.6369	6	7	3	5	7	5	2	301	a
13528.5963	12	4	3	1	3	2	2	240	
13528.7181	13	5	1	5	6	2	4	202	
13528.9766	21	8	2	6	9	3	7	202	a
13536.0645	4	9	4	6	10	3	7	202	a
13539.2550	8	1	0	1	2	2	0	221	a
13541.7638	23	9	3	6	10	2	9	042	
13547.0173	12	3	0	3	4	1	4	320	a
13548.0222	12	7	4	4	8	3	5	320	
13548.1501	11	6	3	4	6	4	3	320	a
13549.0839	5	8	5	3	8	5	4	141	a
13549.3316	43	4	2	3	5	1	4	320	a,b
13550.1341	14	7	1	6	7	4	3	202	a
13556.9353	7	5	2	4	5	3	3	320	a
13557.9578	24	3	1	3	4	0	4	320	a
13559.2264	15	5	3	2	5	4	1	320	a
13560.9115	12	4	3	2	4	4	1	320	a
13561.6113	8	7	2	6	8	3	5	122	a
13562.0700	180	5	5	1	6	5	2	221	a,b
13562.7813	7	5	3	3	6	2	4	320	
13565.9669	25	7	2	6	7	2	5	221	a
13567.3686	10	7	5	2	7	2	5	160	a
13568.6629	21	8	1	7	9	2	8	202	a
13570.6732	18	8	2	7	9	1	8	202	a
13571.0554	118	9	0	9	10	1	10	170	a,b
13573.1144	9	3	2	2	3	3	1	320	a
13574.3754	8	9	3	7	9	3	6	221	a,b
13575.5401	6	7	2	5	7	3	4	320	
13578.6243	13	3	2	1	3	3	0	320	a
13580.1522	9	4	2	2	4	3	1	320	a
13581.7861	12	5	2	3	5	3	2	320	a
13582.8331	9	3	2	2	4	1	3	320	a
13585.1196	7	8	5	4	8	6	3	320	a
13585.2550	40	8	4	5	9	3	6	202	a
13588.7728	29	6	5	2	7	5	3	221	a
13589.8563	88	4	1	4	5	2	3	202	a
13591.2738	6	5	1	4	5	4	1	202	a
13592.8450	5	10	2	8	10	4	7	301	a
13593.2050	50	4	1	4	4	1	3	221	a
13593.5501	10	7	5	2	7	6	2	202	a
13596.1550	15	3	3	1	4	4	0	202	a
13598.4889	10	3	0	3	3	1	2	320	a
13600.8888	13	6	5	2	6	6	1	202	a
13602.5100	5	4	3	2	5	2	3	320	a
13602.5700	40	6	5	1	7	3	4	141	a
13602.8140	24	3	1	2	3	2	1	320	a
13605.0650	5	5	2	4	5	4	1	301	a,b
13605.5610	5	6	3	4	5	4	1	042	a
13605.6412	15	6	3	3	7	2	6	320	a
13606.5275	15	9	0	9	9	1	8	170	a,b
13611.7365	10	1	1	1	2	0	2	320	a
13612.7297	12	2	0	2	2	1	1	320	a
13612.9950	15	8	4	5	8	5	4	202	a
13616.4349	8	2	2	1	3	1	2	320	a
13616.6568	26	5	3	2	6	2	5	320	a
13617.4929	42	8	8	1	8	8	0	301	
13618.6444	19	2	1	2	3	3	1	301	a
13618.7209	31	8	6	3	9	5	4	202	
13619.7215	116	6	3	3	7	1	6	221	a

Note. All transitions originate from the 000 vibrational state.

[a] Assignment confirmed by combination differences.

[b] Lines reassigned from the work of Mandin *et al.* (*2*).

[c] These three lines were incorrectly assigned by Mandin *et al.* (*2*), new assignments have not been made.

TABLE 1—*Continued*

ν (cm^{-1})	Intensity	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	
13619.9331	121	5	5	1	6	5	2	301	a,b
13621.0966	11	1	0	1	1	1	0	320	
13625.8002	8	9	6	4	9	6	3	141	a
13629.3053	7	7	1	7	8	0	8	202	
13630.7761	8	7	2	5	7	5	2	122	a
13632.1127	63	7	3	5	7	3	4	221	a
13632.7228	22	3	2	2	4	3	1	202	a
13633.5150	49	6	4	3	6	5	2	202	a
13636.4843	8	8	5	4	9	4	5	320	a
13636.8825	14	5	2	3	5	4	2	301	a
13637.0550	15	6	2	4	6	4	3	301	a
13637.2098	241	2	1	2	2	1	1	221	a
13639.2089	8	3	2	1	4	1	4	320	a
13642.5361	6	9	7	2	9	7	3	301	
13642.6320	10	9	7	3	9	7	2	301	a
13643.0384	4	3	2	1	2	1	2	042	
13643.3511	13	5	2	3	6	1	6	320	a
13644.0568	58	6	5	2	7	2	5	240	a
13645.3333	13	5	4	1	6	3	4	320	a
13645.5156	4	4	1	4	3	2	1	320	a
13648.8066	26	4	2	2	5	0	5	221	a
13651.8554	7	3	2	1	4	0	4	221	a
13654.4046	8	5	2	3	6	0	6	221	a
13654.6363	71	6	2	4	7	1	7	320	a
13654.9941	7	7	6	1	8	5	4	202	a
13655.2100	7	3	3	0	4	2	3	320	a
13658.9429	6	4	4	0	4	2	3	141	a
13661.2100	4	8	4	5	8	4	4	221	a
13661.9501	6	7	5	2	7	4	3	240	a
13665.3886	6	9	2	7	9	3	6	202	a
13665.5389	11	2	2	0	3	3	1	202	a
13666.4656	3	5	4	2	4	3	1	240	a
13668.3506	23	4	4	1	5	3	2	320	a
13669.0193	4	7	1	6	7	4	3	122	a
13670.7506	11	2	0	2	1	1	1	320	a
13673.2169	25	4	4	0	5	3	3	320	a
13676.5296	9	9	5	4	9	5	5	301	a
13677.5462	18	9	3	7	9	3	6	301	a
13678.7600	6	4	2	2	3	3	1	320	a
13680.0716	10	3	1	2	2	2	1	320	a
13681.4624	4	5	3	2	4	4	1	320	a
13681.8349	39	1	1	1	0	0	0	320	a,b
13688.3465	40	6	1	5	6	3	4	301	a
13689.2826	16	2	1	2	3	2	1	202	a
13692.3513	50	3	0	3	2	1	2	320	a
13693.3081	16	8	3	5	8	3	6	221	a
13694.5366	9	6	3	4	5	4	1	320	a
13696.6762	3	4	1	3	4	4	0	122	a
13702.6650	5	4	4	1	5	5	0	122	a
13702.8527	11	6	5	1	5	5	0	141	a
13705.1324	7	6	3	3	5	4	2	320	a
13706.8975	17	6	4	2	7	3	5	202	a
13707.4431	26	3	1	2	3	3	1	301	a
13708.0706	21	5	2	3	4	3	2	320	a
13708.5954	857	5	5	1	5	5	0	221	a,b
13709.8435	35	7	3	4	7	2	5	320	a
13709.9175	22	3	1	3	2	0	2	320	a
13710.9250	15	4	0	4	3	1	3	320	a
13711.4196	17	5	2	3	6	3	4	122	a
13713.5439	19	8	3	6	8	3	5	301	a
13717.5697	13	8	3	6	7	4	3	320	a
13718.2390	17	6	5	1	7	4	4	202	a
13719.0532	30	5	1	4	5	1	5	221	a
13720.4326	34	8	5	4	7	6	1	202	a
13721.4428	16	7	0	7	8	1	8	122	a
13723.6722	14	4	3	2	5	0	5	320	a
13724.6435	16	7	1	6	6	4	3	202	a
13724.8383	5	3	3	0	2	2	1	042	
13726.0764	55	5	0	5	4	1	4	320	a
13727.1324	10	7	1	7	6	3	4	301	a
13727.4794	11	7	3	4	8	2	7	202	a
13728.4842	8	8	4	5	7	5	2	320	a
13729.6650	15	6	2	4	6	3	3	202	
13731.0778	13	5	1	5	4	0	4	320	a
13731.3428	54	3	2	2	3	3	1	202	a
13731.8455	12	6	4	3	7	2	6	221	a
13732.0264	11	7	2	6	6	4	3	301	a
13732.5178	12	6	1	5	6	2	4	202	a
13732.7430	8	4	3	1	4	0	4	042	a
13734.6676	53	5	1	4	4	2	3	320	a
13735.7736	24	4	2	3	4	0	4	221	a
13736.0080	70	4	1	4	4	2	3	202	a
13736.9850	39	6	2	5	6	1	6	320	a
13737.0688	57	4	2	2	4	3	1	202	a
13737.1619	44	6	2	4	5	3	3	320	a
13738.1996	17	6	0	6	5	1	5	320	a
13738.5500	5	8	4	5	8	4	4	301	a
13740.0882	19	6	1	5	6	1	6	221	a
13740.7410	31	6	1	6	5	0	5	320	
13741.0797	200	3	2	2	4	1	3	202	a
13742.4605	10	4	3	2	3	2	1	042	a
13743.0153	11	8	5	4	8	5	3	221	a
13743.1923	9	8	2	6	8	2	7	221	a
13744.3198	12	7	3	5	6	1	6	141	a
13744.4072	6	8	5	3	7	5	2	141	a
13744.5446	32	8	5	3	8	5	4	221	a
13747.4315	33	2	2	1	1	1	0	320	a
13748.1764	5	5	5	1	6	4	2	202	a
13748.6231	4	5	0	5	4	3	2	202	a
13749.2576	44	8	3	6	7	0	7	240	a,b
13749.7985	102	7	0	7	6	1	6	320	a,b
13750.3869	10	3	2	1	4	3	2	122	a
13752.2302	15	6	2	5	6	0	6	221	a
13753.1318	6	5	1	4	6	2	5	122	a
13753.8839	7	2	2	0	1	1	1	320	
13756.1281	5	8	0	8	7	1	7	320	
13756.3593	8	6	2	5	7	1	6	122	
13758.3833	17	6	1	5	5	2	4	320	b
13759.8623	405	6	5	1	6	5	2	221	a
13762.1237	34	7	2	6	7	0	7	221	a
13763.1596	24	3	2	2	2	1	1	320	a
13763.4600	5	9	0	9	8	1	8	320	
13763.5293	8	7	5	2	7	0	7	160	a
13764.0772	21	4	4	0	5	3	3	202	a
13765.7348	5	10	1	10	9	0	9	320	
13766.4625	792	5	5	1	5	5	0	301	a,b
13769.3908	9	6	3	4	5	2	3	042	a
13770.0794	37	4	1	3	4	2	2	202	a
13770.2450	40	7	3	5	7	1	6	221	a
13772.7900	40	2	2	1	3	3	0	122	a
13773.2904	44	5	0	5	6	1	6	122	a
13774.7283	14	5	4	2	4	1	3	240	a
13775.4212	126	4	2	3	3	1	2	320	a
13776.5446	12	5	1	5	6	0	6	122	
13776.9350	15	2	2	0	1	0	1	221	a
13776.9840	64	10	0	10	9	0	9	221	a
13777.7643	29	10	1	10	9	1	9	221	a
13778.1036	33	7	1	6	6	2	5	320	
13778.2182	5	9	3	7	9	1	8	221	a
13780.0428	19	6	4	3	5	5	0	202	a

TABLE 1—*Continued*

ν (cm^{-1})	Intensity	J"	K_a"	K_c"	J'	K'_a	K'_c	$v_1v_2v_3$	
13780.5270	35	8	5	4	7	6	1	320	a,b
13781.3672	6	10	2	8	10	2	9	221	a
13781.5151	7	6	4	2	5	5	1	202	a
13781.8928	23	11	0	11	10	0	10	221	
13783.4281	24	6	2	4	5	4	1	301	a
13783.9750	5	12	1	12	11	1	11	221	
13784.1055	117	3	3	0	4	2	3	202	a
13784.5577	73	3	2	1	2	1	2	320	a
13785.4117	64	5	2	4	4	1	3	320	a
13785.4991	32	5	4	1	5	3	2	320	a
13785.5550	5	6	4	3	6	3	4	320	a
13786.8017	9	9	2	7	8	0	8	141	
13790.0363	6	5	4	2	5	3	3	320	
13790.2665	6	9	3	6	8	4	5	320	
13793.7300	7	8	1	7	7	2	6	320	
13795.2530	10	7	4	4	6	5	1	202	a
13796.3411	6	8	3	6	7	1	7	141	
13796.7723	14	4	0	4	5	1	5	122	a
13796.8644	114	7	5	2	6	2	5	160	a
13797.1805	30	5	2	3	6	1	6	202	a
13798.0529	103	6	4	3	5	1	4	240	a
13798.2273	20	7	4	3	6	5	2	202	a
13801.9964	20	7	2	5	6	5	2	122	a
13802.1541	13	2	1	1	3	2	2	122	a
13802.4831	20	5	3	3	4	4	0	202	a
13802.9035	7	4	1	3	3	3	0	301	a
13803.8137	9	3	2	1	2	0	2	221	a
13804.2763	11	6	4	3	5	2	4	141	
13805.8607	54	8	3	5	8	3	6	301	a
13806.0428	9	9	1	8	8	2	7	320	
13808.3378	28	8	4	5	7	5	2	202	a
13808.4845	35	2	2	0	3	1	3	202	a
13809.3416	24	7	6	2	6	6	1	141	a
13811.5780	69	0	0	0	1	0	1	071	
13813.9491	11	8	5	4	8	4	5	202	a
13816.2015	13	8	2	6	7	4	3	301	a
13816.5512	21	2	2	0	3	0	3	301	a
13816.6210	9	7	0	7	6	3	4	122	a
13816.8214	9	6	3	4	6	4	3	122	a
13817.0023	93	6	3	4	5	4	1	202	a
13817.2541	49	3	0	3	4	1	4	122	a
13817.9137	40	10	2	9	9	1	8	320	a
13818.0101	34	4	2	3	5	1	4	122	a
13818.1216	66	5	0	5	4	2	2	301	a
13819.1779	49	3	3	1	2	2	0	320	
13820.1720	39	9	1	8	8	1	7	221	
13820.6761	50	3	3	0	2	2	1	320	a
13823.5862	13	9	2	7	8	3	6	320	
13824.2138	11	4	1	4	3	2	1	202	a
13826.3402	46	7	1	6	6	3	3	301	a
13826.4418	23	10	2	9	9	2	8	221	a
13826.8650	52	7	1	7	6	2	4	170	a
13829.6551	60	5	2	4	4	3	1	202	
13829.9054	9	11	1	10	10	1	9	221	
13830.6735	18	7	3	4	7	2	5	202	a
13831.0718	56	8	3	6	7	4	3	202	a
13831.1916	8	8	1	8	7	2	5	122	
13832.5291	46	10	1	9	9	1	8	221	a
13832.6959	143	6	2	5	5	3	2	202	a
13834.9523	7	4	2	3	4	3	2	122	a
13835.1275	16	5	5	0	5	4	1	320	a
13835.1999	6	5	5	1	5	4	2	320	a
13835.4874	6	7	5	3	6	4	2	240	
13835.6909	36	7	4	4	6	2	5	141	
13835.9775	16	2	0	2	3	1	3	122	a
13836.4221	12	7	5	2	6	4	3	240	a,b
13836.7331	11	12	1	11	11	1	10	221	
13836.8630	48	4	3	2	3	2	1	320	a
13838.2647	21	11	2	10	10	2	9	221	
13840.1071	60	8	0	8	7	2	5	071	a
13843.5343	13	7	1	6	6	4	3	122	a
13843.6821	30	4	3	1	3	2	2	320	
13845.4930	12	9	3	7	8	1	8	141	
13845.5693	13	9	6	4	8	6	3	141	a
13846.2349	9	5	5	0	6	6	1	400	a
13847.4872	9	3	2	1	3	3	0	122	a
13848.2530	18	7	2	5	7	3	4	122	a
13851.1848	75	9	3	7	8	3	6	221	a
13852.3574	8	8	0	8	9	0	9	023	a
13853.8301	8	5	4	2	5	2	3	221	a
13855.5044	8	8	5	3	7	4	4	240	
13858.3699	73	6	3	4	5	2	3	320	a
13858.4883	20	9	2	7	8	2	6	221	
13860.3577	12	10	3	8	9	3	7	221	
13860.8743	9	7	3	5	6	2	4	320	
13861.1885	11	6	5	2	6	4	3	042	
13862.0505	33	6	4	2	6	3	3	202	a
13862.5365	8	9	7	3	8	7	2	301	a
13863.8048	17	4	1	3	4	0	4	202	a
13865.7592	40	5	2	3	4	1	4	320	a
13866.3967	52	8	3	6	7	2	5	320	a
13866.9194	113	7	6	2	6	6	1	301	a
13867.7653	12	9	3	7	8	2	6	320	
13868.5544	5	6	3	3	6	0	6	320	a
13869.0380	10	4	1	3	4	2	2	122	a
13869.2063	100	5	3	2	4	2	3	320	a
13869.4829	11	10	3	8	9	2	7	320	
13871.0001	11	11	1	11	10	3	8	023	
13872.3105	65	3	3	0	3	2	1	202	a
13872.8555	152	3	1	2	3	2	1	122	a
13873.0850	5	10	2	8	9	2	7	221	a
13873.1328	87	6	4	3	6	3	4	202	a
13873.2010	32	9	3	6	8	3	5	221	a
13874.0183	9	8	5	4	8	4	5	320	a
13875.0532	16	7	3	5	7	2	6	202	a
13878.2781	8	12	2	10	11	2	9	221	
13878.6924	7	9	3	7	9	2	8	202	a
13880.1450	5	7	1	7	8	1	8	023	a
13880.5548	11	10	2	8	10	2	9	301	a
13880.6560	40	2	0	2	1	0	1	071	
13881.5000	5	8	6	3	7	6	2	301	a
13882.2663	102	7	3	5	7	1	6	301	a
13883.0720	41	2	0	2	2	1	1	122	a
13884.8497	13	2	2	1	3	1	2	122	a
13887.4971	22	10	3	7	9	3	6	221	
13887.8490	30	10	4	7	9	4	6	221	
13888.5945	11	6	1	5	6	0	6	202	a
13888.6801	13	6	2	4	7	2	5	023	a
13895.1242	20	7	1	6	7	0	7	202	a
13895.2511	24	9	6	4	8	6	2	301	a
13895.4370	8	9	6	3	8	6	2	301	
13895.8419	20	5	5	1	5	4	2	202	a
13896.6639	14	5	3	3	6	5	2	103	a
13898.5234	11	6	1	5	7	1	6	023	a
13899.0400	45	6	3	3	5	2	4	320	a
13903.9267	17	10	4	6	9	4	5	221	a
13904.7000	5	10	5	6	9	5	5	301	
13905.5877	5	8	2	7	8	1	8	202	a

TABLE 1—*Continued*

ν (cm^{-1})	Intensity	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	
13908.6492	12	10	6	4	9	6	3	301	
13908.9422	34	8	2	7	8	0	8	301	a
13912.2566	30	4	3	2	3	0	3	320	a
13913.4277	12	4	4	1	5	5	0	400	a
13914.2450	5	9	2	8	9	0	9	301	a
13914.4902	172	6	2	4	5	1	5	320	a
13914.8369	704	5	3	2	4	3	1	301	a
13918.3211	48	6	1	6	5	0	5	202	
13919.9935	12	5	1	4	6	1	5	023	a
13924.9655	11	5	3	3	6	4	2	400	a
13928.5699	437	8	2	6	7	3	5	202	a
13929.1576	45	5	2	4	6	2	5	023	a
13929.6424	23	5	3	2	6	4	3	400	a
13934.7096	10	7	3	5	6	0	6	042	
13939.1323	13	5	4	2	5	2	3	301	a
13939.4377	84	8	1	7	7	2	6	202	a
13939.8749	59	8	5	3	7	5	2	221	a
13941.1572	23	2	0	2	1	1	1	122	a
13941.4423	488	9	0	9	8	1	8	170	a,b
13941.8096	45	4	1	3	5	1	4	023	a
13942.1859	142	9	2	7	8	3	6	202	a
13944.6729	5	3	3	0	3	1	3	301	a
13945.2788	11	10	4	7	9	3	6	320	
13945.5388	116	8	2	7	7	1	6	202	a,b
13945.9614	36	8	4	5	7	3	4	320	a
13946.3858	10	9	4	6	8	3	5	320	
13947.1828	400	10	0	10	9	0	9	301	a
13947.5604	72	8	4	4	7	3	5	042	a,b
13947.7048	36	3	3	0	3	0	3	202	a
13948.1660	66	3	3	1	2	2	0	202	a
13949.0735	51	5	3	3	4	1	4	221	a
13949.6841	11	11	3	9	10	1	10	141	
13949.7985	84	9	3	6	8	2	7	042	a
13950.1216	50	3	1	2	2	2	1	122	a
13950.2261	22	7	2	6	6	3	3	122	a
13950.6700	5	10	1	9	9	2	8	202	a
13951.2253	15	7	5	2	6	3	3	141	
13952.7110	55	7	4	3	6	3	4	320	
13957.1833	26	5	5	1	4	4	0	320	a
13957.3450	60	5	5	0	4	4	1	320	a
13957.8579	14	4	2	2	4	1	3	122	
13959.1321	34	10	3	8	9	3	7	301	a,b
13961.6867	13	7	6	1	6	5	2	320	
13962.4111	10	10	4	7	9	4	6	301	
13962.7643	8	4	1	3	4	0	4	122	a
13963.2011	8	6	3	4	5	4	1	122	a
13972.1061	16	6	3	3	5	4	2	122	
13978.1357	13								c
13979.9400	200	6	5	2	5	2	3	240	a,b
13980.6995	22	5	1	4	5	0	5	122	a
13981.1239	16	4	0	4	3	1	3	122	a
13991.5605	13	8	0	8	9	1	9	400	a
13993.3457	6	7	3	5	8	2	6	400	a
13995.7139	21	5	0	5	4	1	4	122	a
13996.9387	9	7	2	6	8	1	7	400	a
13999.0351	11	9	3	7	10	3	8	103	a
14001.3326	9	7	3	4	6	4	3	122	
14002.3223	8	5	2	4	5	1	5	122	
14002.5963	10	4	2	2	5	4	1	103	a
14005.4264	46	8	5	4	7	4	3	202	a
14007.8320	12	8	7	2	7	6	1	202	
14016.8843	13	10	5	6	9	4	5	202	
14020.6436	15	6	3	4	6	2	5	122	a
14021.4913	24	7	6	2	6	5	1	202	
14021.5634	52	7	6	1	6	5	2	202	a
14022.4096	31	2	2	0	1	1	1	122	a
14024.0569	24	9	4	6	8	3	5	202	
14029.6650	11	8	3	6	9	3	7	103	a
14030.0164	17	9	2	8	10	2	9	103	a
14036.7061	13	9	4	5	8	2	6	221	
14041.6293	53	7	2	5	6	3	4	122	a
14050.2962	20	9	6	3	8	5	4	202	
14054.5834	13	6	4	3	6	3	4	122	a
14061.4972	18	8	4	4	7	3	5	202	
14062.2500	30	10	4	6	9	2	7	221	a
14065.4778	38	8	5	4	7	4	3	320	a
14068.1515	23	5	5	1	4	3	2	221	a,b
14068.8620	5	7	2	6	6	1	5	122	a
14076.0262	16	5	3	2	5	4	1	400	a
14083.1242	21	6	4	2	6	4	3	023	
14086.8605	12	9	5	4	8	4	5	320	
14088.6903	14	9	4	5	8	3	6	202	
14101.3450	5	9	5	4	8	3	5	301	a
14107.9063	19	5	1	5	5	2	4	400	a
14116.4300	5	4	1	3	4	1	4	023	a
14120.4850	5	8	2	6	8	4	5	103	a
14123.7496	18	6	2	4	6	3	3	400	a
14126.0148	17	5	5	1	4	3	2	301	a,b
14129.7620	5	8	1	8	8	1	7	103	a
14142.3470	19	9	5	5	8	3	6	301	
14159.3162	40	4	4	1	3	3	0	122	a
14161.5000	5	9	6	4	9	6	3	103	
14162.2539	9	9	3	7	9	3	6	103	a
14166.5400	5	8	6	2	7	4	3	301	a
14174.8800	5	4	2	2	3	2	1	023	a
14177.0533	34	7	1	7	6	1	6	023	a
14177.7730	5	8	4	4	7	1	7	042	a
14178.3000	5	5	4	2	4	3	1	122	
14179.3600	15	5	4	1	4	3	2	122	
14180.6380	5	4	3	2	3	0	3	122	a
14182.2330	5	8	5	4	7	3	5	221	a
14184.1662	16	9	6	4	8	4	5	301	a
14186.2758	24	8	0	8	7	0	7	023	a,b
14186.8500	5	4	2	2	5	1	5	400	a
14187.4026	17	5	1	4	4	1	3	023	a,b
14193.7967	52	7	2	6	7	2	5	103	a
14194.7558	11	6	4	3	5	3	2	122	a
14198.4824	16	6	2	5	5	2	4	023	
14203.2788	50	6	1	5	5	1	4	023	a
14205.2600	14	1	0	1	2	2	0	103	a
14210.2192	19	7	5	2	7	5	3	103	a
14224.5789	33	6	2	4	5	2	3	023	a
14234.3884	47	5	5	0	4	4	1	122	
14245.7176	8	5	3	2	6	4	3	004	a
14252.1420	5	7	3	4	6	4	3	400	a
14254.6550	13	7	4	4	7	3	5	400	a
14255.4214	26	6	5	2	5	4	1	122	
14255.7200	5	6	5	1	5	4	2	122	
14266.6442	12	7	3	5	7	2	6	400	a
14267.8841	18	8	3	6	8	2	7	400	
14276.2880	14	7	5	2	6	4	3	122	
14278.8850	5	8	3	5	7	3	4	023	
14281.3450	8	6	2	4	5	3	3	400	a
14288.8700	5	6	0	6	5	2	3	103	a
14293.2000	5	7	3	4	7	3	5	103	a
14293.3563	12	7	2	6	7	1	7	400	a
14303.9680	13	9	1	8	9	0	9	400	
14306.9168	26	6	6	1	5	5	0	122	
14325.2934	18	8	0	8	7	1	7	400	a
14326.1086	12	7	6	1	6	5	2	122	

TABLE 1—*Continued*

ν (cm^{-1})	Intensity	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	
14332.1889	9	8	1	7	7	2	6	400	
14335.1956	13	10	1	10	9	0	9	400	
14336.9255	15	7	2	6	6	1	5	400	a
14342.7013	8	10	2	9	9	1	8	400	
14347.3087	9	4	3	1	4	0	4	400	a
14347.8552	13	3	2	1	4	3	2	004	a
14354.3096	19	7	6	2	6	6	1	103	a
14361.0184	32	5	3	2	5	0	5	400	a
14362.1400	10	10	3	8	9	2	7	400	
14363.9072	12	6	2	4	5	5	1	004	
14367.1829	12	6	5	2	5	5	1	103	a
14369.4750	5	4	4	0	3	3	1	400	a
14378.1833	20	7	7	0	6	6	1	400	
14381.2300	17	7	5	2	6	5	1	103	a
14393.0380	9	8	5	4	7	5	3	103	
14394.3200	5	6	3	3	6	0	6	400	a
14395.9400	5	3	3	1	3	1	2	103	a
14397.6238	22	8	1	7	8	1	8	103	a
14397.8928	12	2	1	2	3	2	1	004	a
14406.9493	10	3	3	1	2	0	2	400	a
14417.1700	5	8	0	8	7	3	5	004	
14419.4850	5	4	0	4	5	1	5	004	a
14419.6840	11	9	1	8	8	4	5	004	
14421.5027	42	7	4	3	6	1	6	122	
14422.2118	16	4	1	4	5	0	5	004	a
14422.6146	12	6	4	3	5	2	4	023	
14424.8262	177	6	3	3	5	2	4	400	b
14429.1931	28	8	3	6	7	3	5	103	a
14429.5465	14	9	4	6	8	4	5	103	
14436.1567	64	7	0	7	6	3	4	004	
14436.8112	62	7	5	2	6	4	3	400	
14438.0448	86	9	2	8	8	2	7	103	a
14438.1650	86	10	1	10	9	1	9	103	
14438.2349	234	10	0	10	9	0	9	103	a
14438.8338	41	7	5	3	6	4	2	400	
14439.0457	65	9	3	7	8	3	6	103	a
14440.2447	17	1	1	0	2	2	1	004	a
14441.2143	14	7	6	2	6	5	1	400	
14441.3583	41	7	6	1	6	5	2	400	
14442.3157	28	10	2	9	9	2	8	103	
14442.9322	48	7	1	6	6	4	3	004	b
14450.7652	33	8	1	8	7	2	5	004	
14451.4657	32	7	4	4	6	2	5	023	
14454.3204	70	8	5	4	7	4	3	400	
14456.1468	20	8	5	3	7	4	4	400	
14456.4567	20	8	6	3	7	5	2	400	
14457.0513	9	8	6	2	7	5	3	400	
14458.4437	20	9	2	7	8	2	6	103	
14458.8058	29	10	2	8	9	2	7	103	
14460.2486	31	8	4	4	7	3	5	400	
14460.6866	21	5	3	3	4	0	4	400	a
14465.0666	17	9	4	5	8	2	6	023	
14468.5163	13	9	5	5	8	4	4	400	
14471.4391	30	9	5	4	8	4	5	400	
14474.9433	20	9	3	6	8	3	5	103	
14482.1405	34	4	4	1	3	1	2	400	a
14484.7034	20	10	3	7	9	3	6	103	
14485.5700	22	9	4	5	8	3	6	400	
14488.9405	15	3	1	2	3	2	1	004	a
14494.4992	17	5	4	2	4	1	3	400	a
14494.6247	9	8	3	5	7	2	6	400	
14495.0098	37	4	3	1	3	1	2	103	a
14509.0054	10	2	0	2	2	1	1	004	
14516.0999	22	5	2	3	4	0	4	103	a
14528.4450	5	7	4	4	6	1	5	400	a
14542.6368	16	5	4	1	4	1	4	400	a
14545.6441	8	5	4	1	4	2	2	103	a
14551.3438	23	1	1	0	1	0	1	004	a
14551.5760	14	8	4	5	7	1	6	400	
14553.7652	31	6	4	2	5	2	3	103	a
14555.9186	13	5	3	2	5	2	3	004	a
14557.0016	22	3	2	1	3	1	2	004	a
14567.2550	5	8	3	6	7	0	7	400	a,b
14652.1231	10	6	2	5	5	1	4	004	
15073.6960	15	9	2	8	10	2	9	311	a
15111.0338	9	7	0	7	8	2	6	033	a
15119.8800	9	8	1	8	9	1	9	311	a
15121.3085	12	7	4	3	8	3	6	330	a
15145.7849	9	7	1	7	8	0	8	212	
15173.0842	9	4	1	4	4	3	1	311	a
15177.9248	45	5	3	2	6	3	3	311	a
15178.2501	25	2	1	1	1	1	0	231	a
15200.5410	8	5	4	1	5	5	0	212	a
15208.4483	12	6	1	6	6	2	5	212	a
15219.8482	15	6	1	6	5	1	5	231	
15228.6407	25	4	3	2	4	4	1	212	a
15232.1650	5	8	0	8	7	0	7	231	
15236.8416	9	8	5	3	8	5	4	311	a
15241.6711	8								c
15244.5448	18	7	5	3	7	5	2	231	a
15244.9671	8	7	5	2	7	5	3	231	
15249.7129	8	7	2	5	7	3	4	212	a
15259.1382	8	6	1	5	6	2	4	212	a
15260.6900	7	6	2	4	6	3	3	212	
15265.1570	10	4	2	2	4	3	1	212	a
15267.3390	6	6	2	5	5	2	4	231	
15293.0541	9	8	1	7	7	1	6	231	
15312.0346	8	6	3	4	5	3	3	231	
15328.4950	13	7	3	5	6	3	4	231	
15336.4876	18	5	4	2	4	4	1	231	a
15349.0496	9	5	3	2	4	4	1	212	a
15349.4517	11	8	3	5	8	3	6	311	a
15359.4464	16	6	3	4	5	4	1	212	a
15371.4300	12	5	3	2	4	2	3	330	
15382.7357	16	2	2	0	2	1	1	212	a
15393.3930	8	8	4	4	7	4	3	231	a
15397.3891	15	8	2	6	8	2	7	311	a
15398.1779	11	7	3	4	6	4	3	212	
15400.5370	16	5	1	4	5	0	5	212	a
15401.8602	25	4	1	3	3	2	2	212	a
15404.3173	8	5	1	5	6	1	6	033	a
15408.0800	13	4	2	3	4	1	4	212	a
15412.3730	13	3	3	0	3	2	1	212	a
15415.7840	14	7	5	3	6	5	2	231	a
15416.3764	12	4	3	2	4	2	3	212	a
15432.1822	8	8	5	3	7	5	2	311	a
15433.9490	21	7	2	6	7	0	7	311	a
15434.0884	19	7	3	4	6	2	5	330	
15436.9714	7	5	4	2	4	3	1	330	
15440.5851	7	8	2	7	8	0	8	311	a
15443.0919	24	7	2	5	6	3	4	212	a,b
15445.7052	28	6	1	5	5	2	4	212	a
15451.5012	18	5	3	3	4	1	4	231	a
15451.8430	14	3	1	3	4	1	4	033	a
15460.3770	22	7	2	5	6	1	6	330	
15461.2512	12	3	2	2	4	2	3	033	a
15466.3685	15	2	0	2	3	0	3	033	a
15475.0417	31	8	2	7	7	2	6	311	a
15478.4584	33	7	4	3	6	3	4	330	a
15486.2322	10	8	3	5	7	2	6	330	

TABLE 1—*Continued*

ν (cm^{-1})	Intensity	J''	K_a''	K_c''	J'	K_a'	K_c'	$v_1v_2v_3$	
15488.4366	8	4	4	0	5	4	1	033	a
15491.1806	18	7	0	7	6	2	4	033	a
15497.4089	11	1	1	1	2	1	2	033	a
15497.5015	22	8	3	5	7	1	6	231	
15509.0038	9	5	4	1	4	2	2	231	a
15510.1930	9	10	3	8	9	3	7	311	
15510.9150	6	0	0	0	1	0	1	033	
15520.7901	9	5	2	4	5	2	3	033	
15524.9573	26	8	3	6	7	2	5	212	
15525.2413	16	7	3	5	6	2	4	212	
15526.7171	15	9	3	6	8	3	5	311	
15534.5331	12	1	1	1	1	1	0	033	a
15542.2100	6	8	4	4	7	2	5	231	a
15542.2814	10	7	0	7	8	0	8	410	
15549.4650	5	3	2	2	3	2	1	033	a
15557.9893	20	2	2	0	2	2	1	033	
15572.1643	9	6	1	6	7	0	7	410	
15573.3003	35	6	4	3	5	3	2	212	
15579.3576	21	2	0	2	1	0	1	033	a
15579.8846	8	4	3	1	4	3	2	033	
15581.0293	15	3	3	1	3	3	0	033	
15581.4090	5	3	3	0	3	3	1	033	b
15583.5355	9	7	4	4	6	3	3	212	
15588.3548	15	8	4	5	7	3	4	212	
15593.7848	11	2	1	1	1	1	0	033	
15597.1954	18	3	1	3	2	1	2	033	a
15597.7200	5	3	0	3	2	0	2	033	
15600.2430	5	5	1	5	6	0	6	410	
15610.6601	13	4	4	0	4	4	1	033	a
15612.5619	9	4	1	4	3	1	3	033	
15613.0755	17	4	0	4	3	0	3	033	
15619.1856	9	3	1	2	2	1	1	033	
15626.7214	19	5	1	5	4	1	4	033	a
15631.0126	7	4	2	3	5	1	4	410	a
15631.4442	14	6	2	4	7	2	5	113	a
15638.9635	13	6	4	2	5	2	3	311	a
15641.5234	8	5	5	1	5	5	0	033	
15643.0211	15	4	1	3	3	1	2	033	b
15647.7050	12	7	1	7	6	1	6	033	
15658.3600	12	4	2	2	3	2	1	033	
15683.0400	9	6	1	5	5	1	4	033	
15709.6070	8	6	2	4	5	2	3	033	
15712.7712	6	8	1	7	7	1	6	033	
15784.3150	5	6	6	0	6	6	1	113	
15789.7920	11	6	5	1	6	5	2	113	
15794.3553	9	2	1	2	1	0	1	410	a
15796.6625	29	5	5	1	5	5	0	113	
15812.0281	21	4	3	2	4	3	1	113	a
15812.6226	10	5	3	2	5	3	3	113	a
15872.7019	15	4	1	3	4	1	4	113	a
15924.6041	14	5	4	2	4	4	1	113	a
15932.7715	8	5	3	2	4	3	1	113	a
15937.6822	17	4	4	1	3	3	0	410	
15937.8600	19	6	2	5	5	2	4	113	
15938.0672	10	7	3	5	6	1	6	033	
15956.6631	9	5	4	2	4	3	1	410	
15957.5627	15	5	4	1	4	3	2	410	
15959.2177	17	8	2	7	7	2	6	113	
15965.8809	15	9	2	8	8	2	7	113	
15967.3399	52	6	2	4	5	2	3	113	a
15973.7584	19	6	4	3	5	3	2	410	
15981.3307	11	7	2	5	6	2	4	113	
15994.9600	5	8	2	6	7	2	5	113	
16004.8850	10	8	3	5	7	3	4	113	

transitions. The strongest unassigned line has a peak absorption of 23%, meaning that there was still a factor of 50 between the strongest and weakest unassigned lines.

The first step in our assignments therefore was to generate 300-K absorption spectra in the range 13 200–16 500 cm^{-1}, using both ZVPT and PS linelists. These were then compared with the experimental spectra starting from the strongest transitions. Tentative assignments were made by comparison with the computed linelists and then confirmed by looking for a further transition associated with the same upper state. Transitions confirmed by these combination differences gave new energy levels that were then used to look for further trivial assignments.

RESULTS AND DISCUSSION

Table 1 presents our newly assigned lines in the 13 200–16 500-cm^{-1} region. Frequencies for these transitions have been taken electronically from the HITRAN database (*10*). Intensities are those measured by Mandin *et al.* (*2*) and are in units of tenth of a percent of peak absorption. A full list of transitions, both unassigned and assigned by them, is given by Mandin *et al.*

Table 1 contains 701 newly assigned lines. The majority of these lines, 487, have, as indicated, been confirmed by combination differences. These assignments can be therefore be regarded as secure. The remaining 214 line assignments were obtained only from direct comparison with the linelists. While we believe these assignments to be correct, they must naturally be regarded with more caution.

Our assigned transitions come from 22 different vibrational bands of $H_2{}^{16}O$, five of which have not been previously observed. Table 2 summarizes the data obtained for each vibrational band; the results of Mandin *et al.* are also summarized. We have not systematically rechecked all Mandin *et al.*'s assignments, however we found 38 lines that had to be reassigned on the grounds of combination differences and other considerations. These lines are also given in Table 1 and the summary of Mandin *et al.*'s data in Table 2 has been adjusted to allow for them. We found three weak lines, which are given in Table 1, were incorrectly assigned by Mandin *et al.* but have so far defied our attempts to reassign them.

Looking at our new vibrational bands we determine the (240) and (033) are weaker bands arising from the 4ν and $4\nu + \delta$ polyads, respectively, and are the sort of band one

TABLE 2

Summary of the Line Assignments Made by Mandin *et al.* (*2*) and Us to the Near Infrared Water Vapor Spectrum of Mandin *et al.*

Band	ν_0(cm^{-1})	Mandin *et al*			This work			
		lines	levels	mis	lines		levels	
					b	c		
160		-	-		4	-	1	
240	13205.1[a]	-	-		10	10	14	d
141	13256.2[a]	42	21	6	12	7	8	
042	13453.7[a]	12	3	3	8	8	9	d
320	13640.8[a]	17	8	1	95	27	57	d
221	13652.656	217	70	5	50	19	25	
170	13661.3[a]	-	-		5	-	2	d
202	13828.277	189	69	3	74	13	18	
301	13830.938	330	100	6	43	8	10	
071	13835.372	-	-		2	2	3	d
122	13910.896	42	24	4	44	16	28	d
023	14066.194	68	38	4	14	7	12	
400	14221.161	176	58	1	29	22	24	
103	14318.813	238	76		26	9	12	
004	14537.5[a]	50	32		10	8	9	
330	15108.1[a]	3	1		2	5	6	d
231	15119.029	92	46	1	8	8	9	
212	15344.503	99	54	3	16	8	10	
311	15347.956	211	81		12	2	3	d
033	15534.709	-	-		14	19	26	d
410	15742.795	36	21		2	7	7	d
113	15832.765	105	51		7	9	10	d

Note. For each band the number of line assignments made and energy levels determined are given for both the previous and this work. The number of misassigned lines, ''mis,'' found in the work of Mandin *et al.* is also given.

[a] Estimated vibrational term value (see text).

[b] Assignments confirmed by combination differences.

[c] Assignments made only by comparisons with calculated linelists.

[d] Term values for these states given in Table 3.

would expect to be responsible for weak transitions at near infrared wavelengths. Conversely, although (170) and (071) belong formally to the $4\nu + \delta$ polyad, one would have anticipated that transitions to states with seven quanta of bend would be too weak to be observed at the sensitivity of the Kitt Peak spectra. However, it transpires that the transitions we assign to these states, all but two of which have been confirmed by combination differences, are isolated ones that steal intensity from nearby ''bright'' states. Such interactions are included automatically in the variational calculations used to construct the linelists used here. As these interactions are localized we would not expect to find further transitions involving these vibrational bands. One level at 14 349.776 cm^{-1} was found to be involved in four distinct transitions. By comparison with the PS linelist, this level was tentatively assigned as $(160)7_{52}$.

Also given in Table 2 are vibrational term values (''band origins'') for 21 of the vibrational bands for which we make assignments. For 14 of these bands, transitions have been assigned that involve the 0_{00} state of vibrational state concerned. In these cases it is possible to quote observed band origins. In particular we find the previously unobserved (071) and (033) band origins at 13 835.72 and 15 534.71 cm^{-1}, respectively. For the other seven vibrational states no transitions involving the 0_{00} state have been assigned. In these cases the band origin cannot be determined directly from the observed data, but it is possible to estimate the band origin using the values given by the PS linelist corrected for the systematic errors relative for observed rotationally excited members of the band. This method of obtaining band origins should be accurate to about ±0.1 cm^{-1}. For (240), (042), and (170) these results represent the first experimental estimates of the band origin. For the (320) state, reassignments, confirmed by combination differences, lead us to the conclusion that the band origin lies 1.4 cm^{-1} lower than the value quoted in Table 1 of Mandin *et al.* (*2*). Estimated band origins for the (141), (004), and (330) states are given by Rothman *et al.* (*10*). Our improved values are consistent with theirs for (141) but are 1 cm^{-1} higher for the (004) and (330) states.

Table 3 presents water energy levels obtained from our and Mandin *et al.*'s data. Results are presented only for vibrational states for which there is a significant amount of new data. Included in this tabulation are results for the (071) vibrational states. Recently, we assigned a number of transitions to the (061) – (050) and (071) – (060) systems in sunspot spectra of hot water (*7*). Since there was no previous data on the (050), (060), (061), or (071) vibrational states, we were unable to extract energy levels for these states from our assignments. The new assignments to the (071) vibrational bands in principle give us a handle on this problem. So far there are insufficient assigned transitions to build a reliable set of energy levels for the vibrational states. However, we are undertaking further work on hot water spectra both in the $(v_1, v_2 + 1, v_3 + 1) - (v_1, v_2, v_3)$ region and the region dominated by bending transitions of the sort $(0, v_2 + 1, 0) - (0, v_2, 0)$, see (*3*). In particular, hotter laboratory spectra should hopefully be sensitive to bands involving (060). These studies should lead to the elucidation of the energy levels of these and other states containing significant bending excitation.

Although we have assignments for nearly all the unassigned transitions of Mandin *et al.*, 132 lines remain unassigned. All these transitions are weak. Although we are confident that, particularly with further experimental input, we will in due course assign all the $H_2{}^{16}O$ transitions in this spectrum, it must be remembered that transitions belonging to $H_2{}^{18}O$ are also present in the spectrum. It is likely that about a half of our unassigned transitions actually involve $H_2{}^{18}O$. Of course $H_2{}^{18}O$ spectra can also be analyzed using the linelist techniques employed here, but as yet we do not have the equivalent linelists for this system. We intend to address this problem in future work.

TABLE 3

Energy Levels of Water (in cm^{-1}) Obtained from the Wavenumbers of the Near Infrared Water Vapor Spectrum of Mandin *et al.* (2)

J	K_a	K_c	033	320	122	311
0	0	0	15534.7093		13910.8965	15347.9561
1	0	1		13663.4678	13933.7842	15370.4209
1	1	1	15576.9043	13681.8271	13950.9199	15383.6943
1	1	0			13956.7998	15389.1562
2	0	2	15603.1299	13707.9053	13978.2559	15413.9482
2	1	2		13722.0928	13990.8467	15423.1924
2	1	1	15636.1562		14008.4600	15439.5459
2	2	1		13789.7998	14058.2158	15479.1309
2	2	0	15692.8906	13791.0195	14059.4990	15480.5000
3	0	3	15667.8096	13771.8447	14042.0918	15476.2207
3	1	3	15676.6807	13780.0098		15481.6943
3	1	2	15714.3613	13814.9766	14085.0107	15514.0586
3	2	2	15761.6211	13858.3330	14126.9473	15546.6328
3	2	1		13864.0430	14132.9053	15552.9170
3	3	1	15866.4482	13955.3408	14223.5400	15626.5293
3	3	0	15866.6279	13955.5723	14223.6934	15626.7461
4	0	4	15749.8369	13853.2002	14123.4023	15556.8945
4	1	4	15754.8398	13857.6709	14127.6328	15556.9277
4	1	3	15816.3857	13914.3535	14184.8164	15611.1748
4	2	3		13948.7891	14217.4648	15635.3887
4	2	2	15870.5156	13963.9941	14233.3535	15651.7930
4	3	2		14049.0186	14317.4033	15719.0146
4	3	1	15962.4014	14049.9834	14318.4736	15720.3877
4	4	1		14177.1602	14444.7344	15828.1406
4	4	0	16098.7666	14177.1816		15828.1660
5	0	5		13950.9141	14220.5518	15651.8438
5	1	5	15851.5586	13953.1299	14223.2412	15652.5469
5	1	4		14035.0273	14306.0527	15728.7266
5	2	4	15967.2998	14060.9102	14328.9473	15744.4805
5	2	3		14090.6074	14360.3867	15776.3984
5	3	3		14165.5547		15834.2227
5	3	2		14169.5674	14438.2529	15839.4746
5	4	2		14294.0039	14562.1416	15944.6348
5	4	1		14294.3105	14561.8760	15944.7861
5	5	1	16383.5986	14445.3174		16090.2959
5	5	0		14445.4521	14722.4961	16090.3486
6	0	6		14064.8242		15764.6289
6	1	6		14066.0879	14336.4609	15764.4775
6	1	5	16082.4971	14174.5918		15864.4932
6	2	5		14184.2354	14460.5732	15872.9785
6	2	4	16156.1172	14241.1152		15924.8223
6	3	4		14304.8740	14573.5547	15971.9004
6	3	3		14315.2490	14582.2188	15985.1816
6	4	3		14434.5332	14703.5615	16084.0283
6	4	2				16085.4707
6	5	2			14865.7617	16231.4150
6	5	1			14865.8330	16231.8799
6	6	1			15048.9922	
6	6	0				16340.7471
7	0	7	16093.9541	14197.0498	14465.5986	15892.1709
7	1	7	16094.9570			15893.0586
7	1	6		14331.0146	14600.2588	16018.5518
7	2	6			14611.7744	16020.1973
7	2	5		14417.8975	14690.6094	16094.7930
7	3	5	16385.3184	14463.6484		16131.5508
7	3	4		14492.2520	14758.0566	16157.6562
7	4	4		14598.1787		16246.9609
7	4	3		14601.6895	14868.7549	16250.8994
7	5	3				16395.8691
7	5	2			15033.0117	
7	6	2		14850.2852		16506.6133
7	6	1			15214.7070	
8	0	8				16038.7949
8	1	8			14613.6006	16039.0703
8	1	7	16416.9844	14503.3379		16182.9756
8	2	7				16184.6504
8	2	6				16282.9932
8	3	6		14648.8066		16309.2383
8	3	5				16355.5781
8	4	5		14788.3184		16433.2500
8	4	4				16442.0234
8	5	4		14996.7148		
8	5	3				16492.0176
9	0	9		14507.6221		16201.6006
9	1	9				16201.6465
9	1	8		14619.6426		16365.9941
9	2	8				16367.3330
9	2	7		14829.7021		
9	3	7		14850.6768		16508.0449
9	3	6		14912.9746		16576.8730
9	4	6		14996.5430		16641.0684
9	5	4		15209.5693		
10	0	10	16381.1143			16381.1143
10	1	10	16381.1113	14685.9033		16381.1113
10	1	9	16566.3926			16566.3926
10	2	9	16567.0371	14896.9893		16567.0371
10	2	8				
10	3	8	16726.4238	15071.4043		16726.4238
10	3	7				
10	4	7		15228.1982		
11	0	11	16577.3223			16577.3223
11	1	11	16577.4062			16577.4062
12	0	12	16790.3027			16790.3027

J	K_a	K_c	410	113	240	042
0	0	0	15742.7939	15832.7637		
1	0	1	15765.2480	15855.4746		
1	1	1	15778.7979	15867.7725		
1	1	0	15784.2969	15873.4004	13269.2686	
2	0	2	15808.7246	15899.3193		
2	1	2	15818.1484	15907.6729	13302.2646	13546.7588
2	1	1		15924.4814		
2	2	1	15874.7266	15961.0088	13414.1797	
2	2	0		15962.5381		
3	0	3	15870.9580	15961.8262		
3	1	3	15876.3867	15966.7607		
3	1	2	15909.0293	15999.7979		13645.6484
3	2	2		16030.9238		
3	2	1	15947.9307	16037.0400		13722.5342
3	3	1		16103.9717		
3	3	0	16020.7744	16104.2500		13859.7402
4	0	4	15950.1396	16041.2227		
4	1	4	15952.8438	16041.3242		
4	1	3		16097.5361		
4	2	3	16030.4844	16123.0000		
4	2	2	16049.0879	16137.6787		
4	3	2	16113.2666	16195.8701	13734.8975	13954.6074
4	3	1	16111.4268	16197.6094		13954.7930
4	4	1	16223.0996	16296.8086		
4	4	0		16296.8760		
5	0	5	16045.7109	16137.1104	13524.0566	
5	1	5	16046.9395	16137.6729		
5	1	4	16123.1592	16215.1445		

Note. Results are only given for vibrational states for which we have made a significant number of new assignments. These levels incorporate those quoted by Mandin *et al.*

TABLE 3—*Continued*

J	K_a	K_c	410	113	240	042
5	2	4		16224.3516		
5	2	3		16263.9121		
5	3	3		16310.7002		
5	3	2	16238.9082	16316.5830		14076.1230
5	4	2	16340.5049	16412.7148	14050.2246	
5	4	1	16340.0791	16413.1797		
5	5	1		16538.7383		
6	0	6		16249.6553		
6	1	6	16158.4072	16250.0078		
6	1	5		16350.1221	13774.9678	
6	2	5		16354.0684		
6	2	4		16413.8496		
6	3	4				14215.9014
6	3	3		16461.4902		
6	4	3	16482.5703	16551.9199	14197.5098	
6	4	2		16553.9141		
6	5	2			14426.4502	14617.9131
6	5	1		16678.3906		
6	6	0		16829.3711		
7	0	7	16286.3447	16379.0596		
7	1	7		16378.4092		
7	1	6		16501.2031	13941.7227	
7	2	6		16502.9551		
7	2	5		16584.1035		
7	3	5		16608.1094		14381.4062
7	5	3			14593.2666	
7	5	2			14593.1465	
8	0	8		16524.5547		
8	1	8			13933.6992	
8	1	7		16668.4766		
8	2	7		16668.8262		
8	2	6		16777.3691		
8	3	6			14335.5010	
8	3	5		16847.2402		
8	4	4	14764.2539			14764.2539
8	5	4			14783.2480	
9	0	9		16688.0820		
9	1	9		16688.1016		
9	1	8				
9	2	8		16851.4805		
9	3	6	14835.3984			14835.3984
10	0	10		16868.0957		
10	1	10		16868.0508		

J	K_a	K_c	071	170
0	0	0	13835.3721	
2	0	2	13904.4502	
7	1	7		14429.6377
8	0	8	14622.5166	
9	0	9		14685.6055

CONCLUSIONS

A significant fraction of the high-resolution near infrared water vapor spectrum of Mandin *et al.* (*2*) has remained unassigned in the literature for over a decade. By use of linelists based on high-accuracy variational calculations, we have successfully assigned over 80% of the unassigned lines in this spectrum. This has led to the first information on five vibrational states and values of the vibrational band origin for four other states. This demonstrates that the technique of assignments based on variational calculations, which we had successfully applied to the spectra of hot water at a number of longer wavelengths (*3–7*), is equally applicable to short wavelength spectra of room temperature water.

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